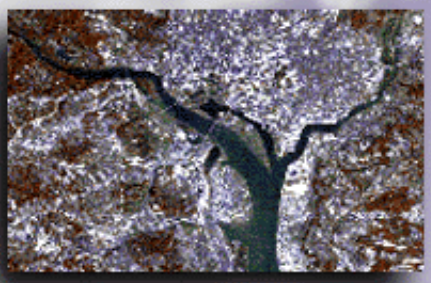
DOE CBNP TRANSPORT & FATE



Argonne
Lawrence Berkeley
Livermore
Los Alamos
Pacific Northwest
Sandia

LA-UR-xxxx

THE MULTI-SCALE MODELING APPROACH

- **The airflow and dispersion problem in CBNP applications involve three spatial scales:**
  - **(1) Single to few building scale (few kilometers, minutes)**

    Individual buildings are explicitly resolved
  - **(2) Many building scale (tens of kilometers, few hours)**

    Clusters of buildings are represented but not individual buildings
  - **(3) Urban scales (> 100 kilometers, many hours)**

    Buildings cannot be resolved and must be para-meterized
- **Customized models with appropriate scale-dependent physics are used for each scale and data is transferred between the scales**

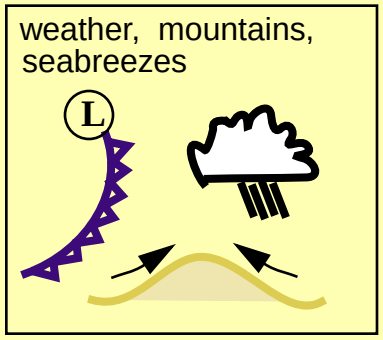
THE CNBP PROGNOSTIC/CFD MODELS

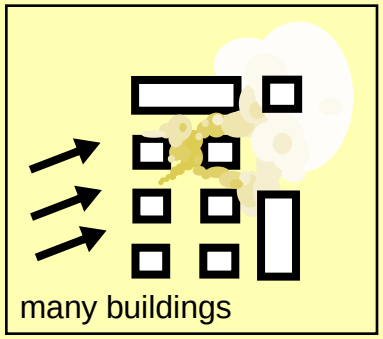
- **Few building scale - FEMCB/MP (developed at LLNL)**
  Typical grid resolution for CBNP applications: 1 m - 10 m

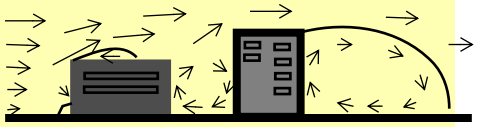
- **Many building scale - HIGRAD (developed at LANL)**
  Typical grid resolution for CBNP applications: 10 m - 100 m

- **Urban/Regional scale - COAMPS (developed at NRL)**
  Typical grid resolution for CBNP applications: > 1 km

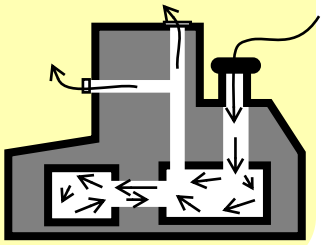
DOE CBNP Multi-scale Modeling







individual buildings, urban canyons



indoor air flow

FLUID DYNAMICS MODELS

MESOSCALE

COAMPS

BC's

URBAN SCALE

HIGRAD

BC's

BUILDING SCALE

FEM3MP

BC's

IN-BUILDING SCALE

GASFLOW
COMIS
SES

DEFINES TRANSPORT

PLUME DISPERSION MODELS

MESOSCALE

LODI

IC's

URBAN SCALE

HIGRAD

IC's

BUILDING SCALE

FEM3MP

IC's

IN-BUILDING SCALE

GASFLOW
COMIS
SES

DEFINES FATE

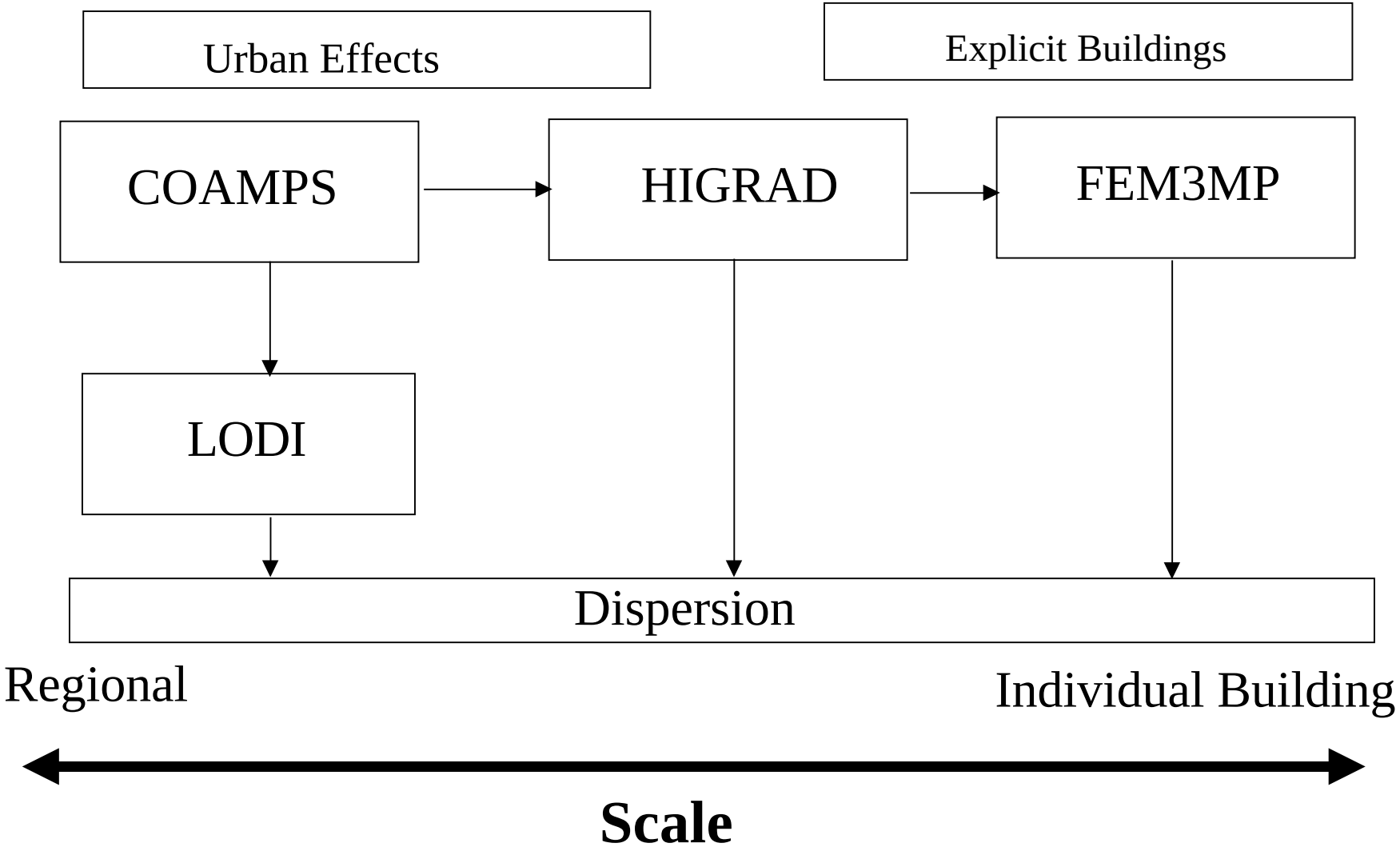
SOURCE TYPE

BIOLOGICAL AGENT

CHEMICAL AGENT

LANL-LLNL

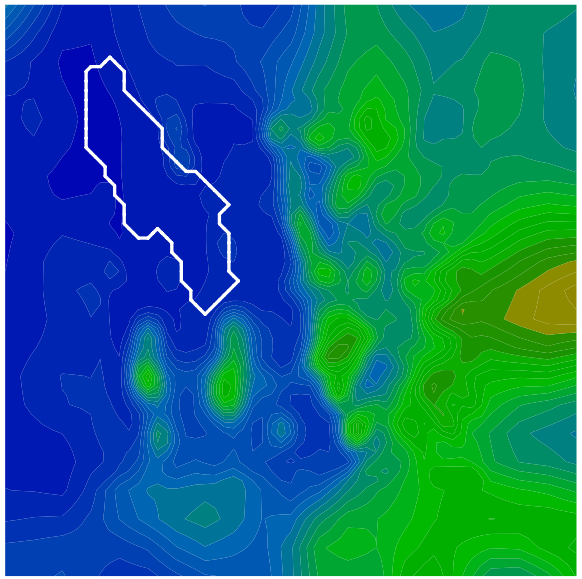
The integrated multi-scale modeling approach

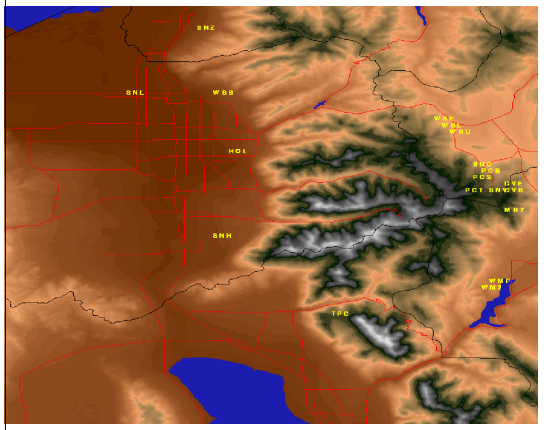


The scales of the models overlap

COAMPS

FEM3MP





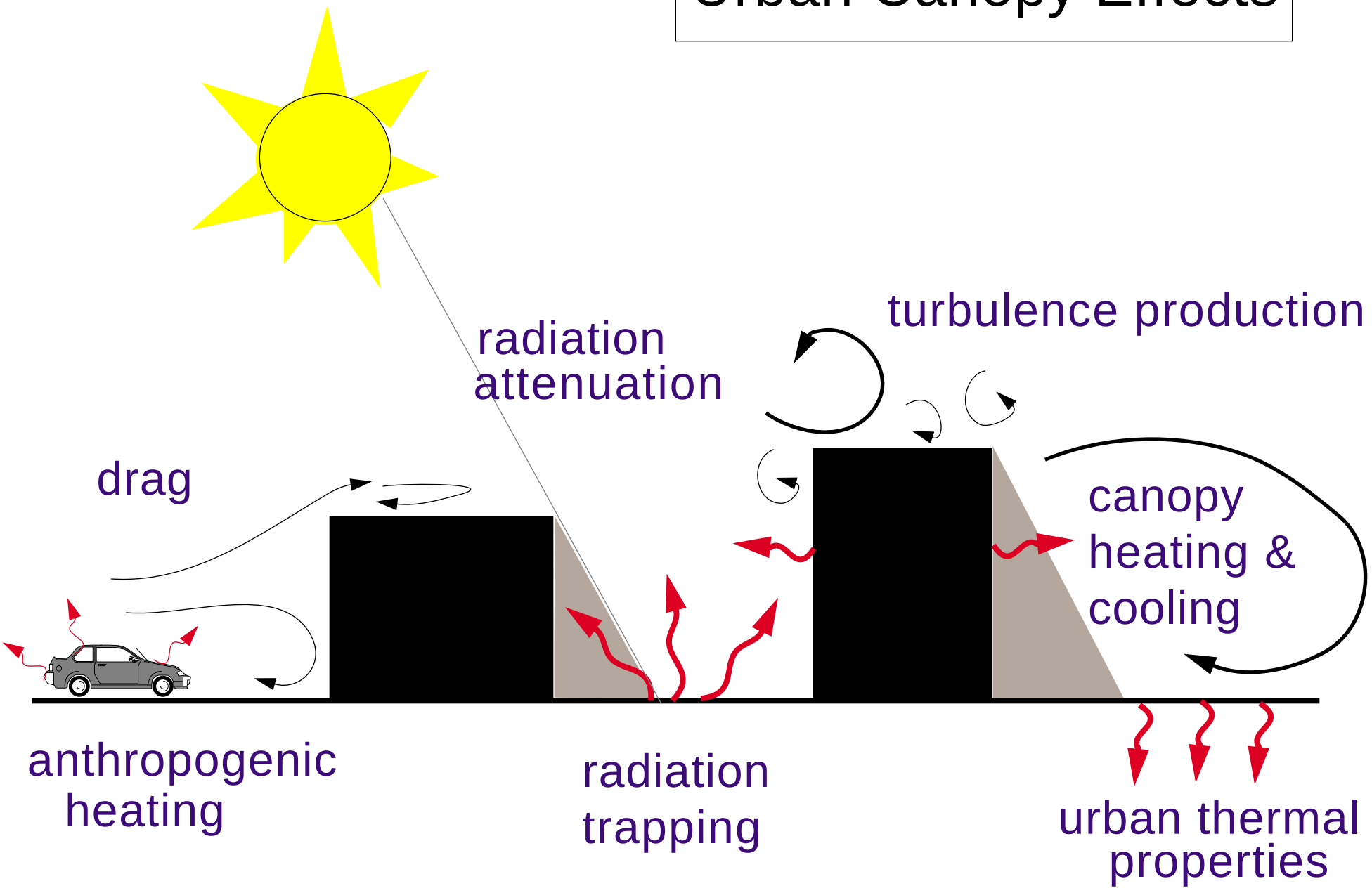
HIGRAD

Regional **Scale** Individual Building

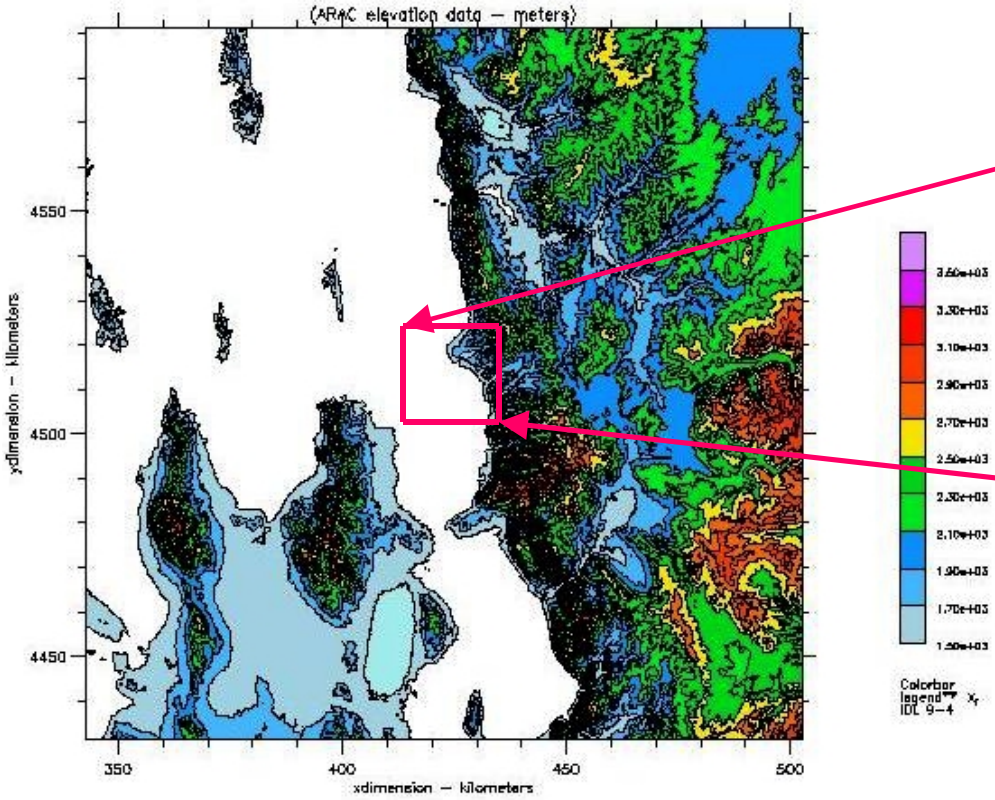
Testing the Urban Parameterization: COAMPS simulations of a hypothetical city

- 36 hour forecasts with and without the urban parameterization
- Initial conditions from NOGAPS, Dec 7 1999 at 1200 GMT (0500 MST)
- Three nests centered at Salt Lake City (40.78N, 111.888W), Δx=36,12 & 4 km
- Salt Lake City is represented as an idealized city
- The results are used to drive the dispersion model, LODI
- The results are also given to HIGRAD and FEM3MP teams for them to derive IC

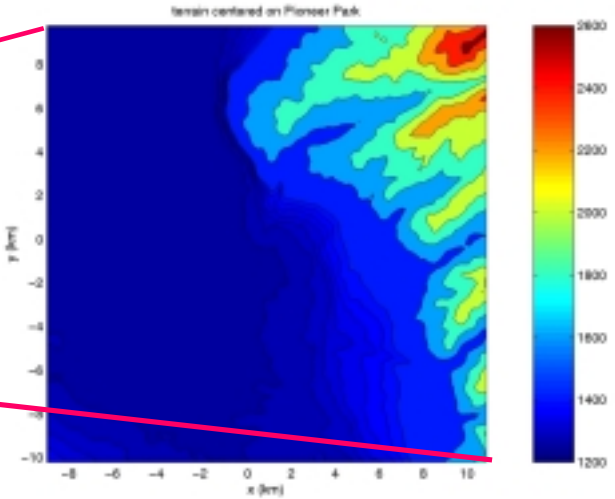
Urban Canopy Effects



TERRAIN IS IMPORTANT AT URBAN SCALE

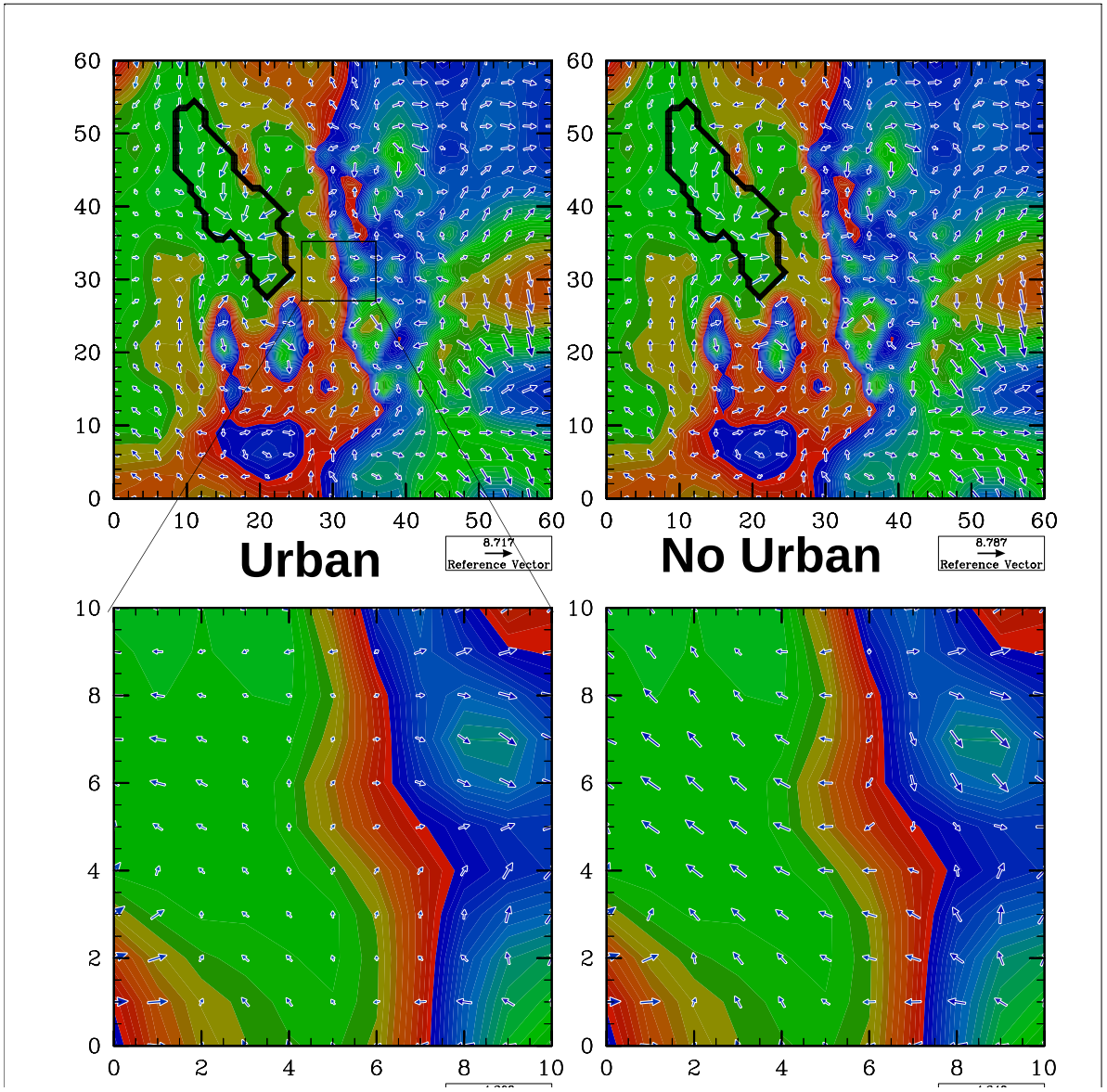


TERRAIN AROND SALT LAKE CITY AREA



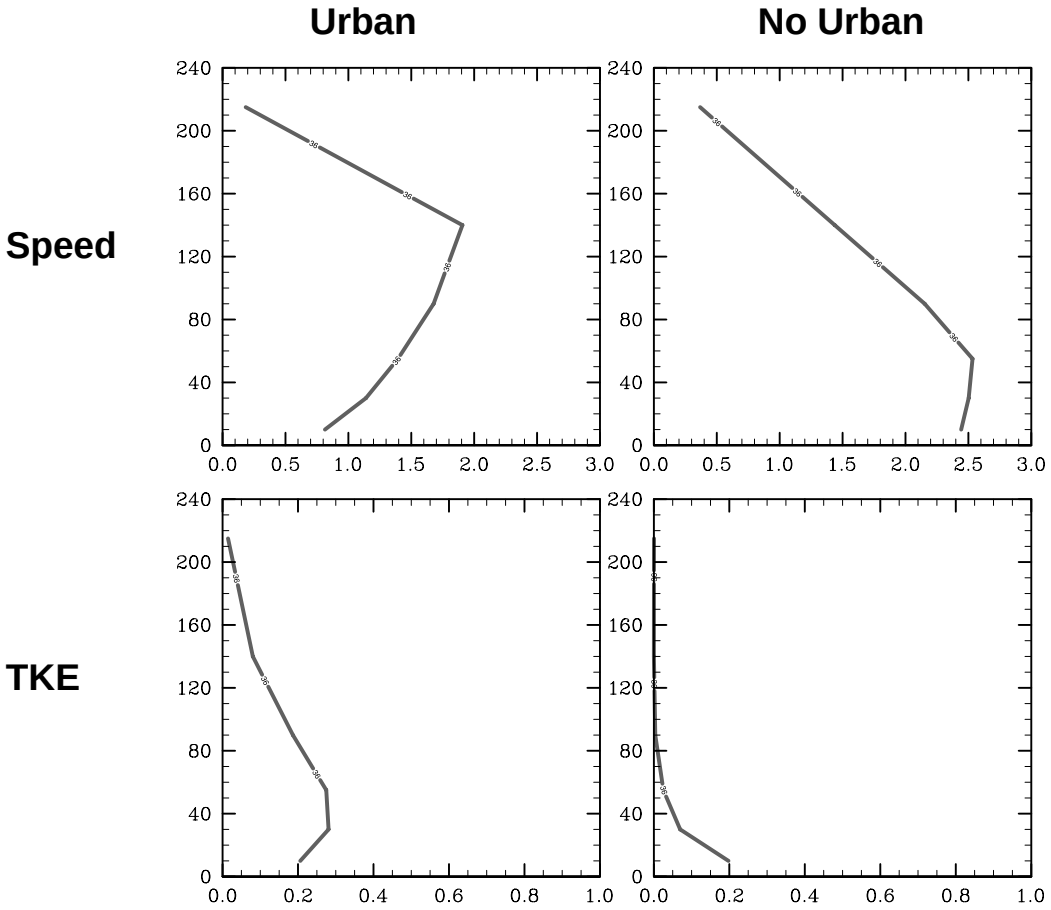
20 km x 20 km DOMAIN CENTERED AT DOWNTOWN SLC SHOWING THE SIGNIFICANCE OF TERRAIN AT THE URBAN SCALE

The urban area modifies the transport winds



The Urban area disrupts the drainage flow

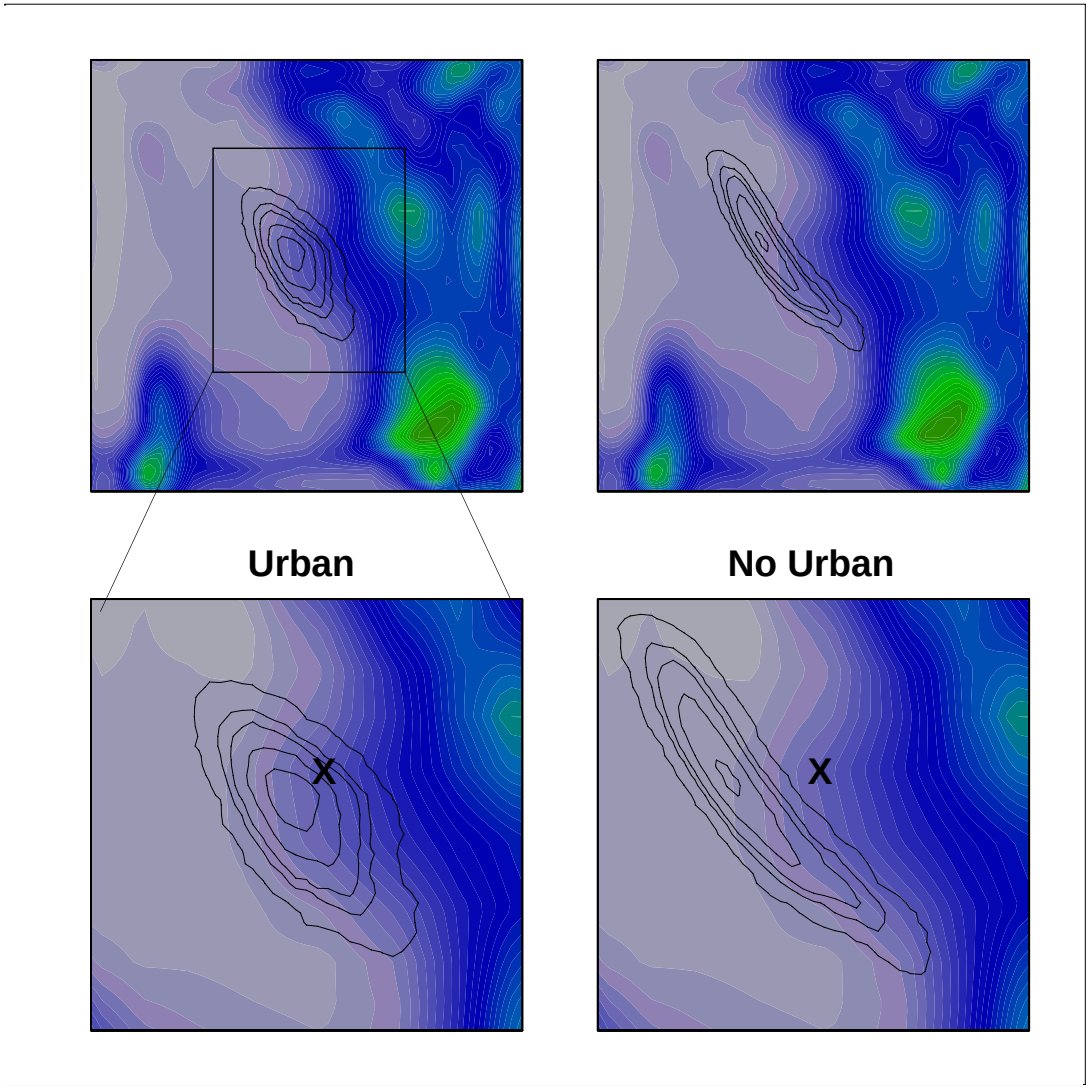
The effects of the urban area are evident in the wind and turbulence profiles



Close to the ground, the wind speed is less and turbulence is greater with the urban parameterization

Changes in the wind speed and pattern and turbulence level alter agent dispersion

Concentration at 3 hours



MANY BUILDING MODEL (HIGRAD)

- Computational Fluid Dynamics (CFD) code with meteorological framework
- Finite difference approach with terrain-following coordinates
- 2nd order numerics in space and time (MPDATA advection scheme)
- Computes on ASCI's massively parallel platforms & Beowulf clusters
- Current model physics:
  - Neutral (chem-bio) agents
  - Full radiation model
  - Surface heating and shading
  - Precipitation microphysics
  - LES turbulence model (Smagorinsky and tke)

Modeling and Prediction: The Many-Building Problem

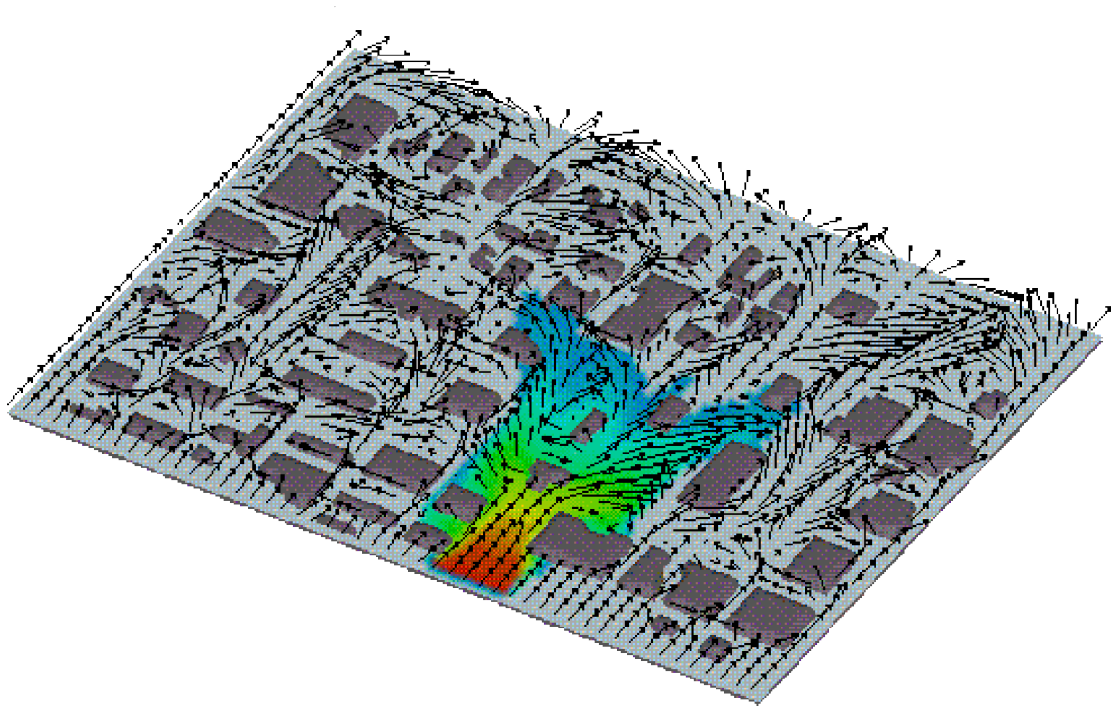
HIGRAD

- **High-gradient, advanced numerics 3D CFD code**
  - **–flow fields around obstacles and sharp corners**

Engineering CFD
+ radiation ✓
+ land use
+ soil moisture
+ ….

↓

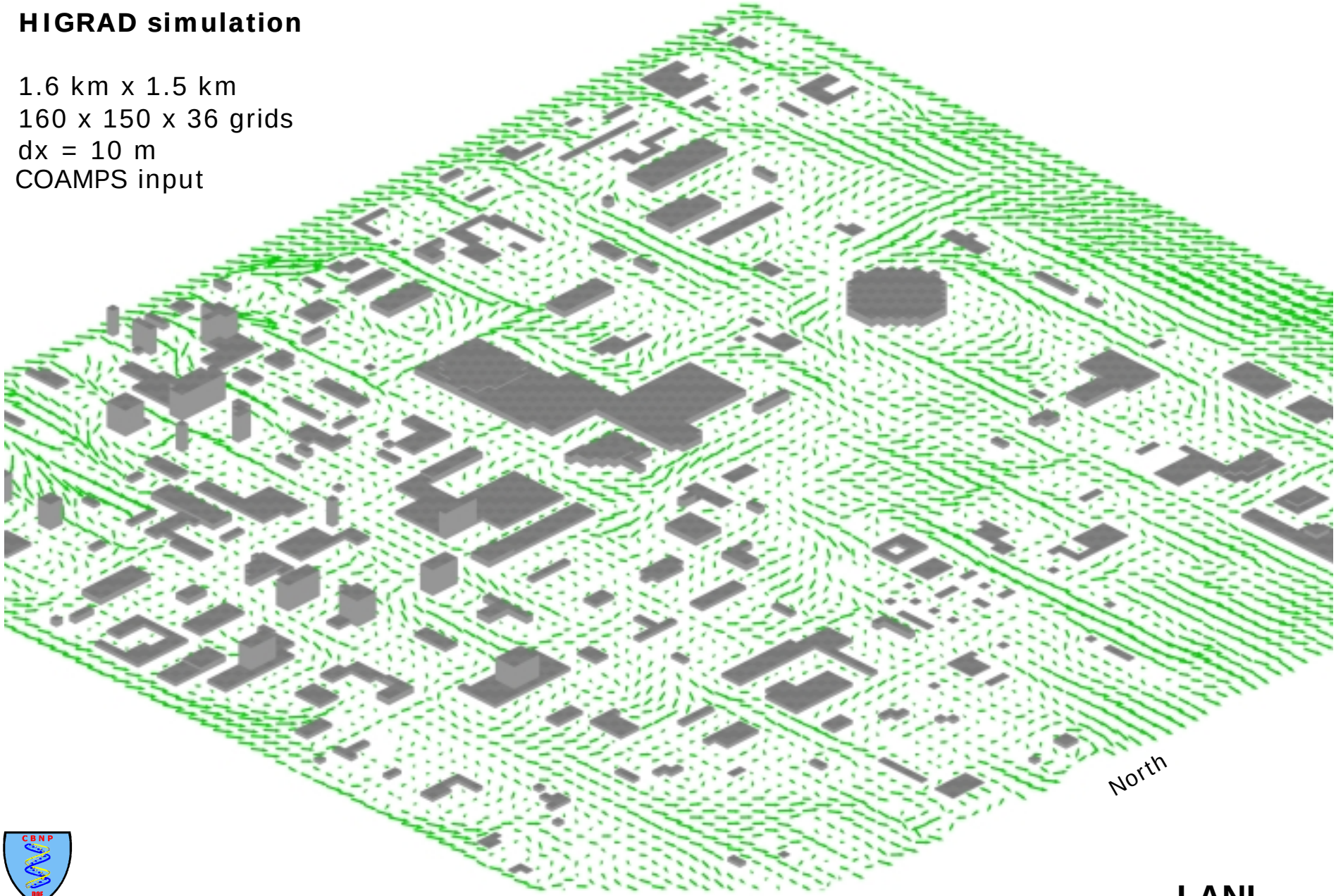
Meteorological CFD



Multi-Scale Modeling

HIGRAD simulation

1.6 km x 1.5 km
160 x 150 x 36 grids
dx = 10 m
COAMPS input

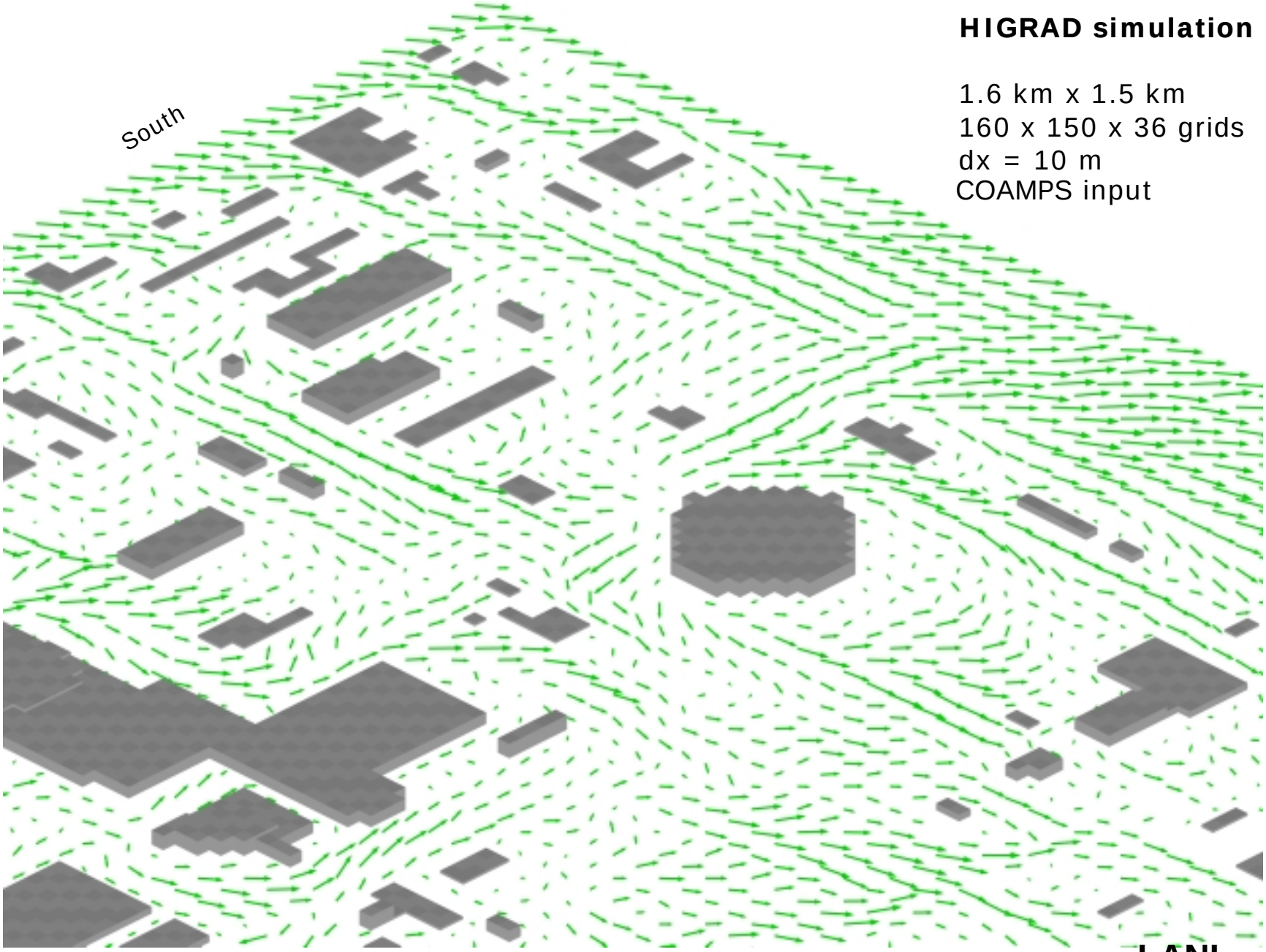


LANL

Multi-Scale Modeling

HIGRAD simulation

1.6 km x 1.5 km
160 x 150 x 36 grids
dx = 10 m
COAMPS input



LANL

Multi-Scale Modeling

HIGRAD simulation

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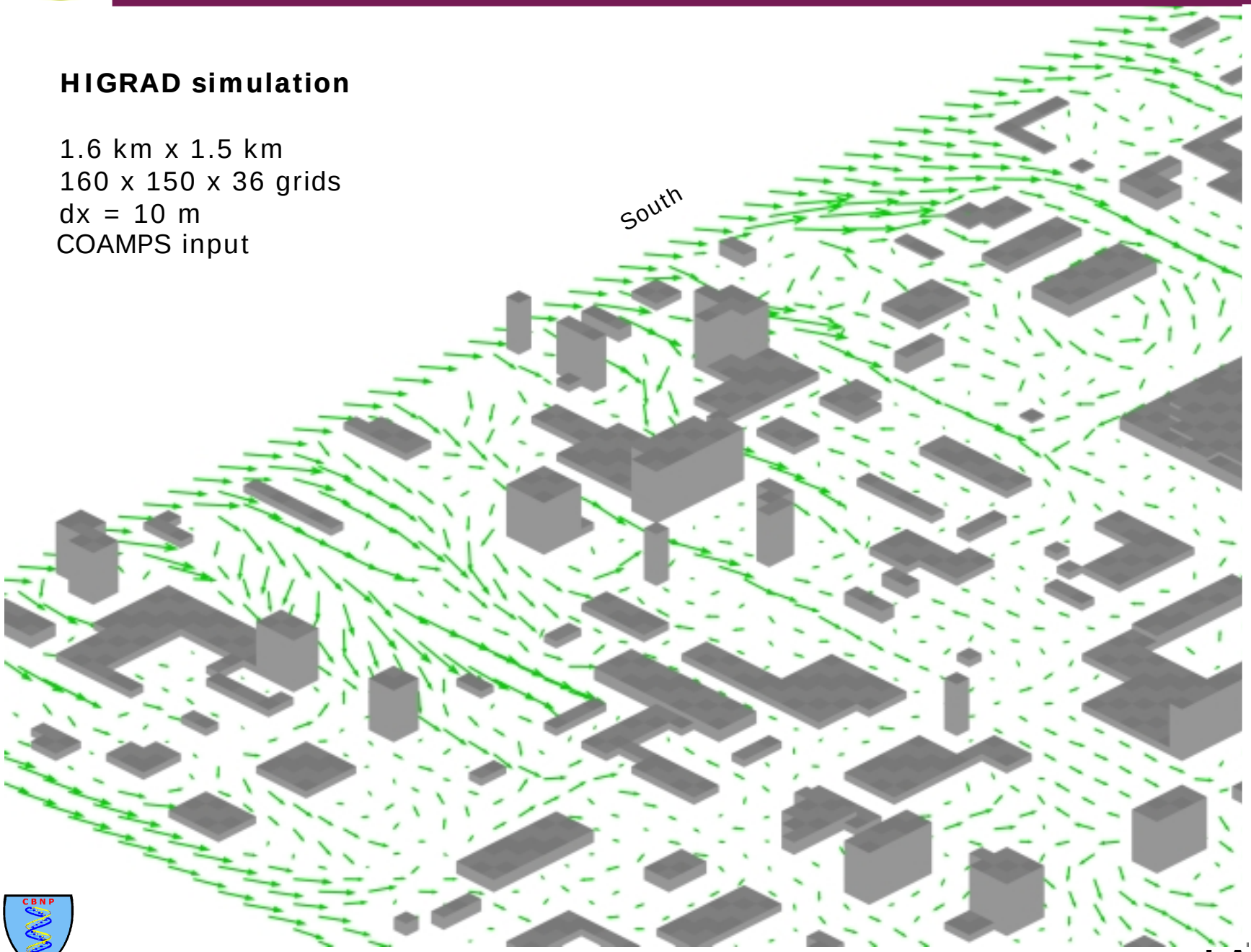
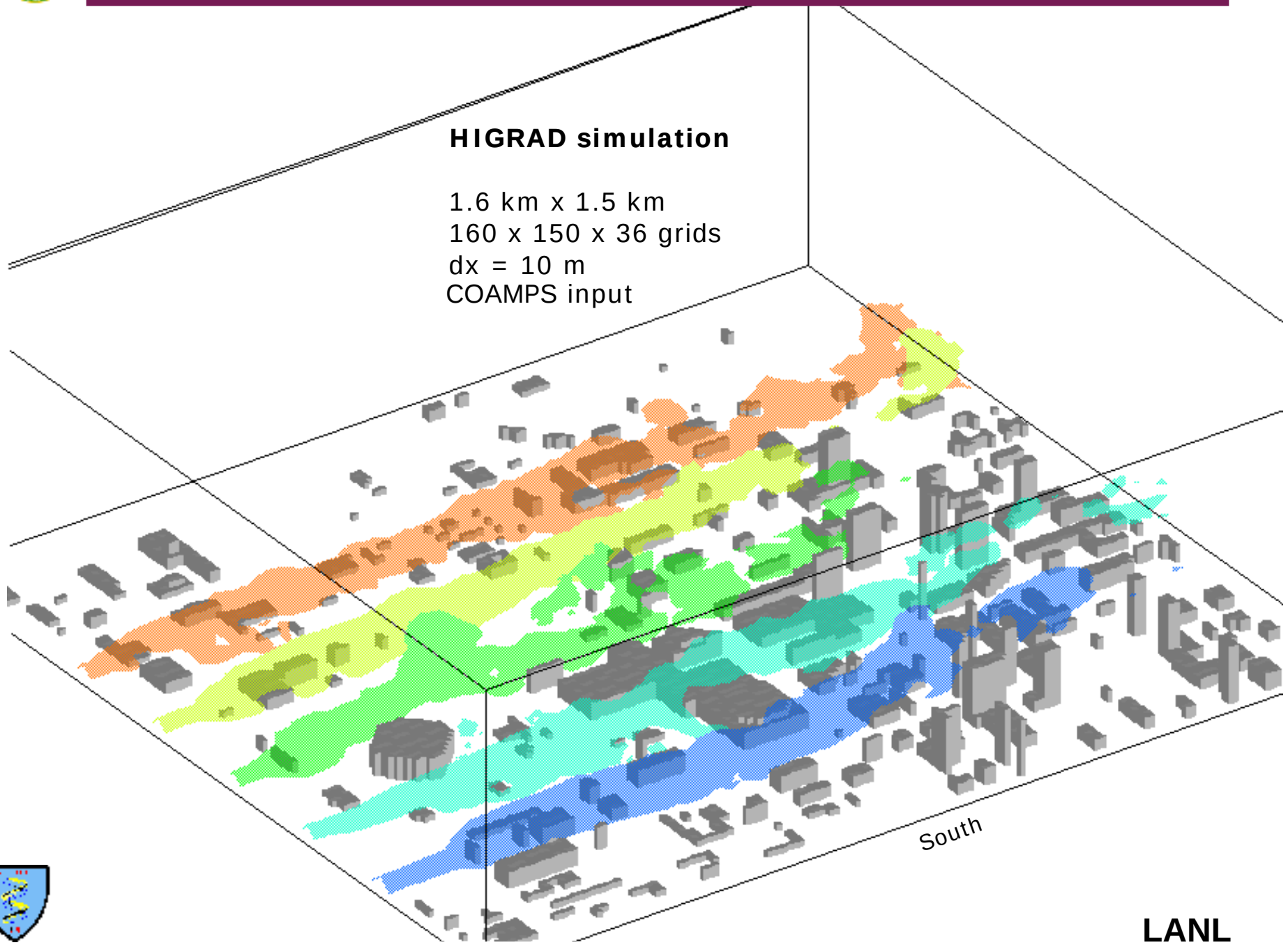


LANL

Multi-Scale Modeling



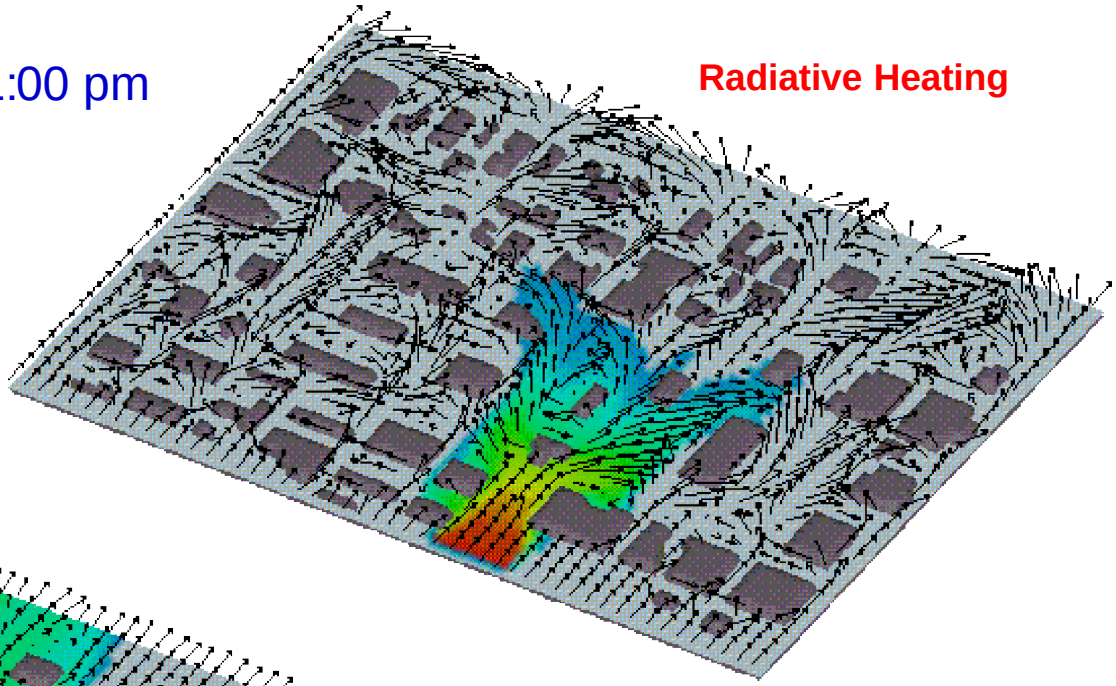
LANL

Modeling and Prediction: The Many-Building Problem

Radiative Heating and Transport

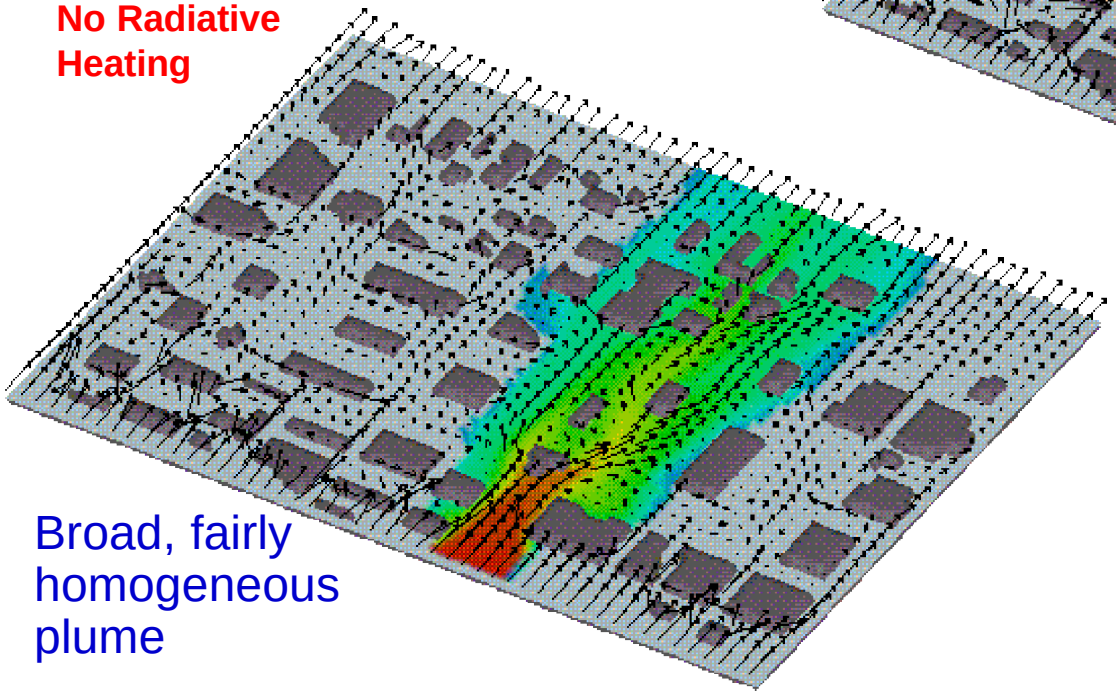
Time-integrated tracer patterns @ 1:00 pm

Radiative Heating



Plume bifurcates and lofts

No Radiative Heating



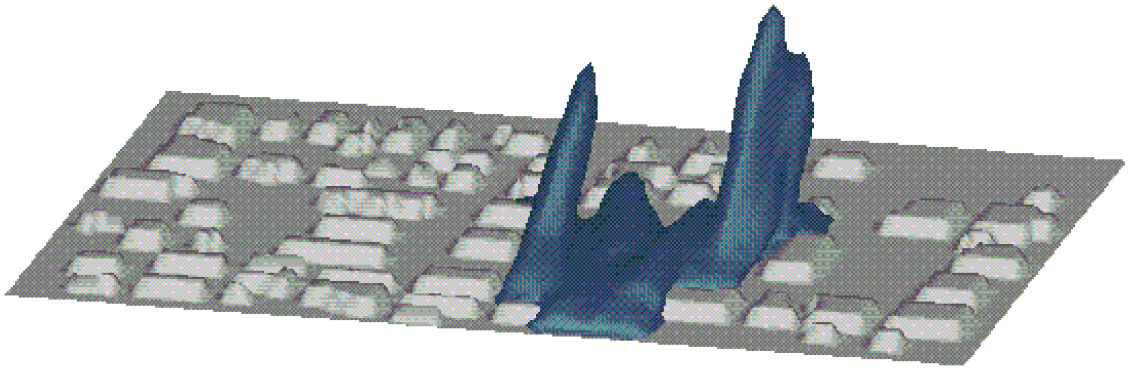
Broad, fairly homogeneous plume

Modeling and Prediction: The Many-Building Problem

Radiative Heating and Transport

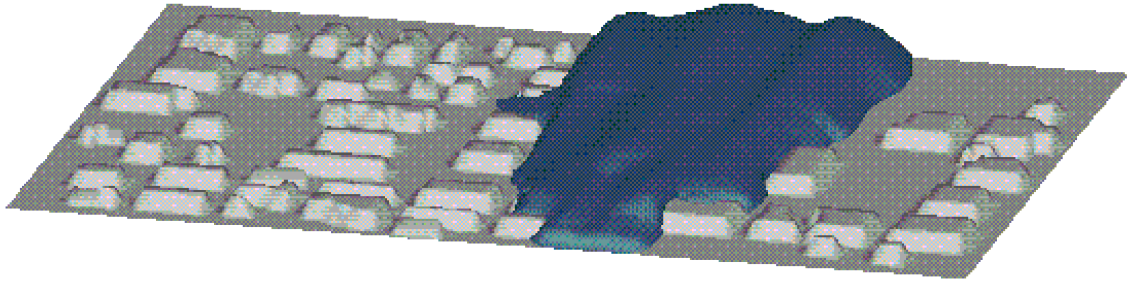
Time-integrated tracer patterns @ 1:00 pm

Radiative Heating



Plume bifurcates and lofts

No Radiative Heating



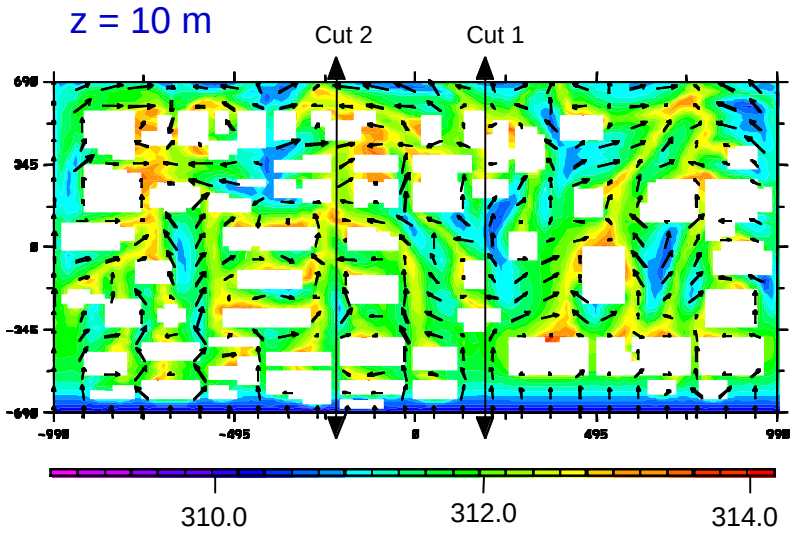
Broad, fairly homogeneous, low-lying plume

Los Alamos National Laboratory

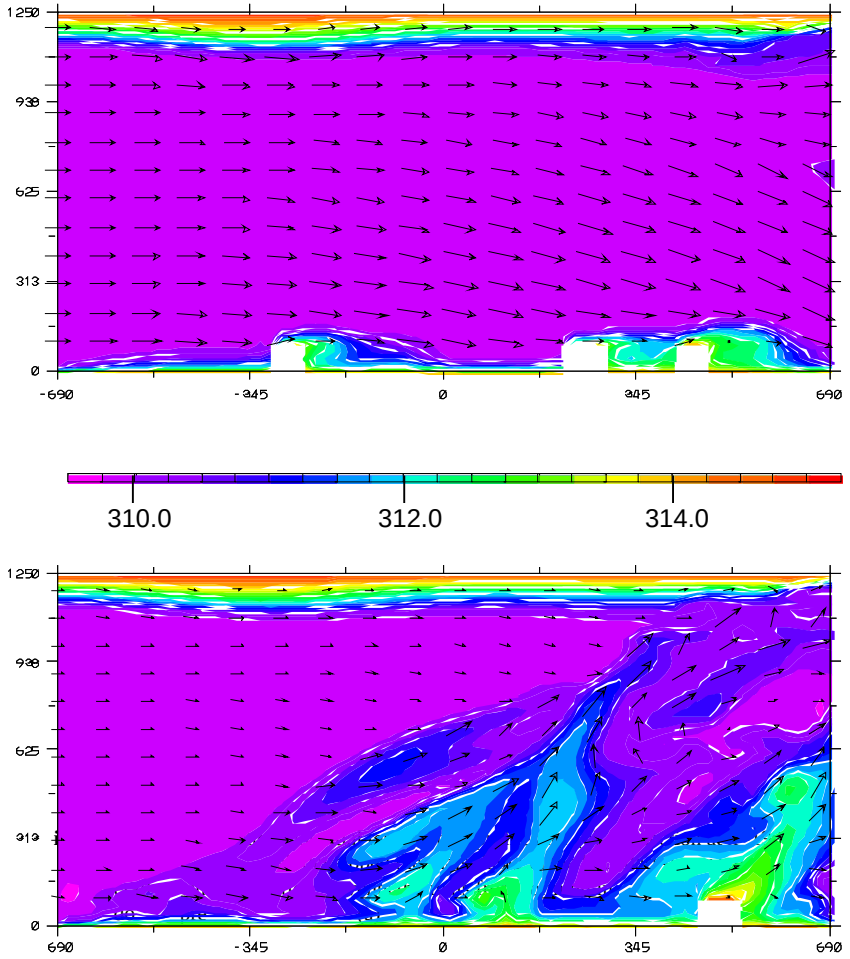
Modeling and Prediction: The Many-Building Problem

Implementation of Radiation Package

Potential Temperature @ 1:00 pm



Vertical x-sections



Cut 1

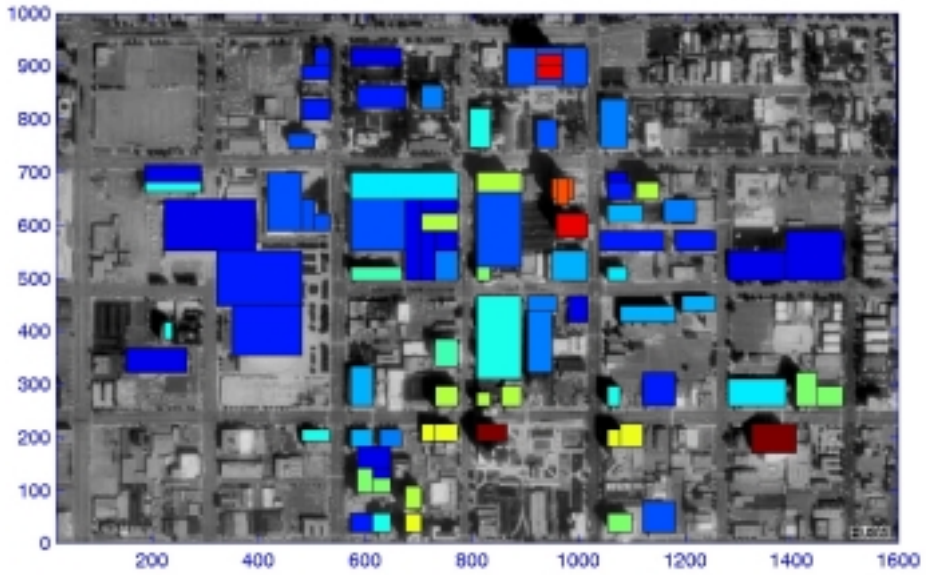
Cut 2

FEW BUILDING MODEL (FEM3CB/MP)

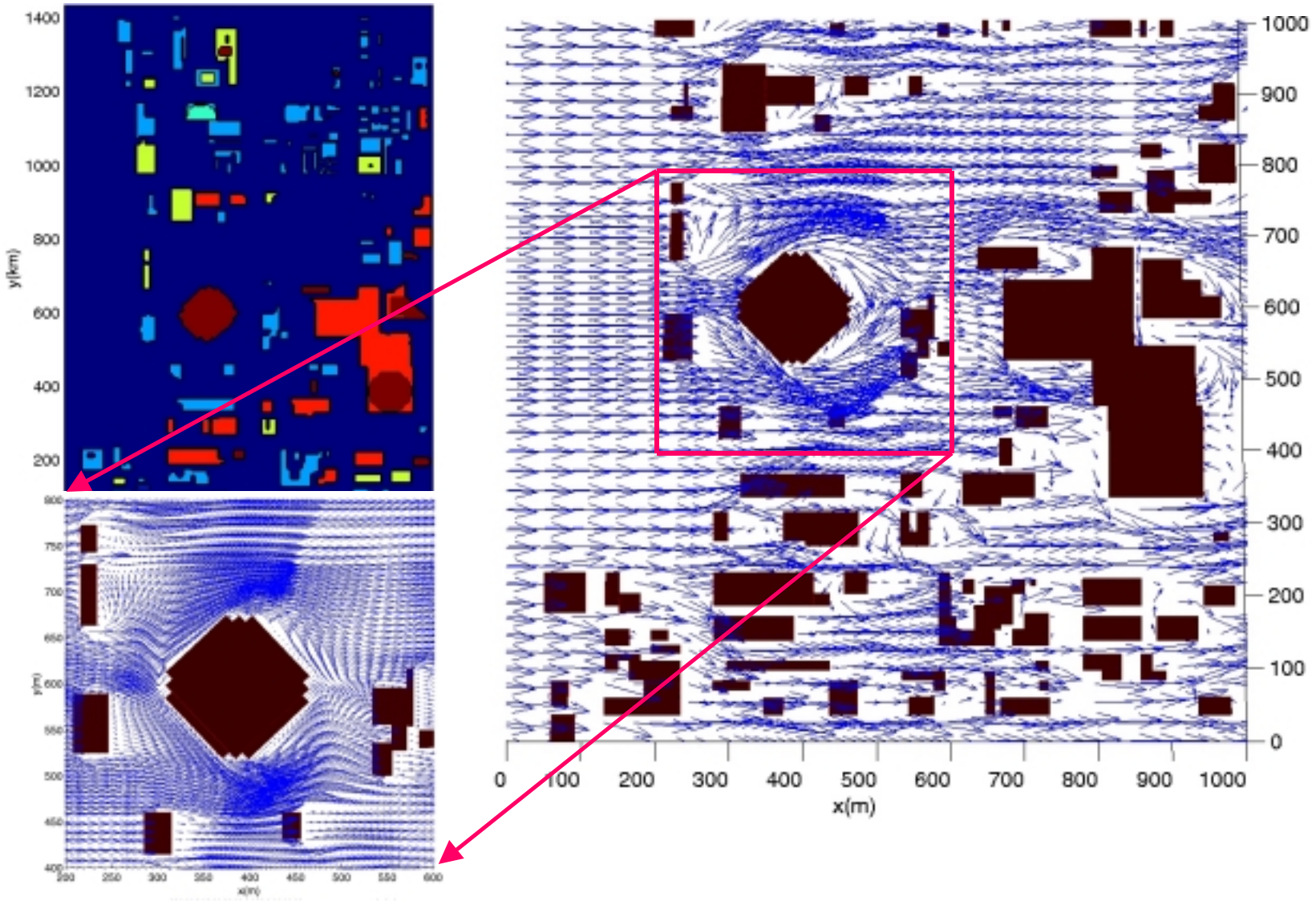
- Computational Fluid Dynamics (CFD) code based on the finite element approach
- Flexible grid system capability including variable resolution, distorted meshes and explicit representation of terrain
- Capability of resolving individual buildings in great detail or few buildings at varying resolutions
- Computes on ASCI's massively parallel platforms
- Current model physics:
  - Neutral (chem-bio) or heavier-than-air (chemical) agents
  - Aerosol physics
  - Surface heating and shading
  - Tree canopy parameterization
  - Reynolds-averaged (RANS) and Large Eddy Simulation (LES) turbulence models
  - First order UV degradation submodel

SIMULATIONS OF FLOW AND DISPERSION AROUND CBNP FIELD OBSERVATION AREA

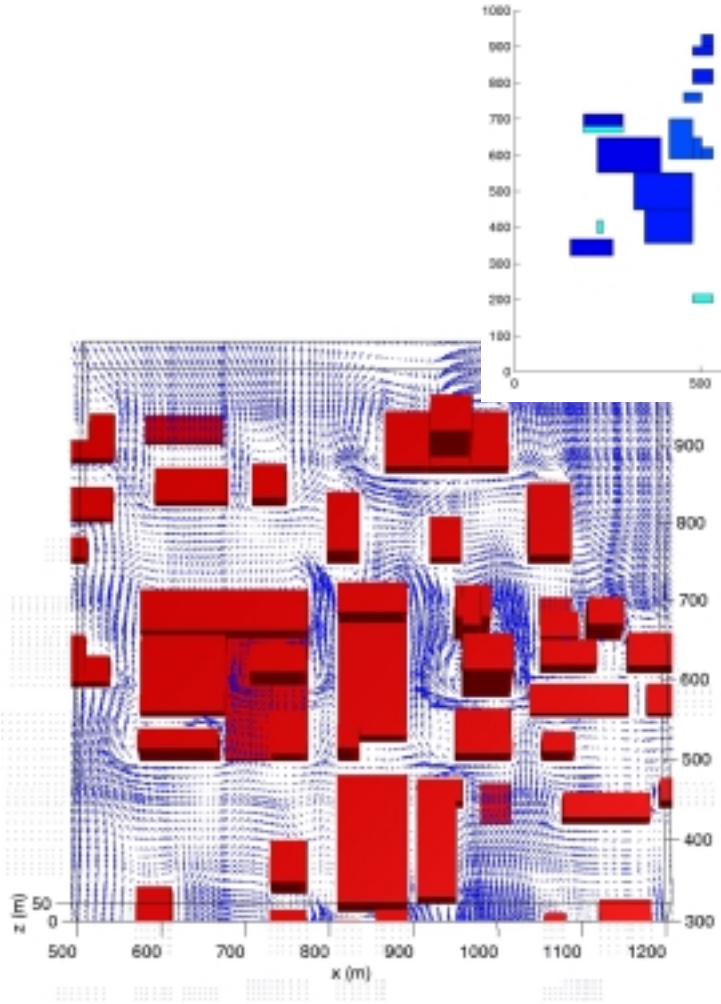
- **Atmospheric conditions:**
  - **Southeast wind**
  - **Wind profile taken from HIGRAD calculation**
  - **Neutral stability**
- **Graded finite element mesh:**
  - **Building locations from satellite photos (heights from shadows)**
  - **Domain size - 2.4 km x 2 km x 300 m**
  - **Grid size - 1.2 million grid points (200 x 148 x 40)**
  - **Minimum grid resolution - 2 m**
- **Release scenario:**
  - **Instantaneous surface releases**
  - **3 downtown locations**



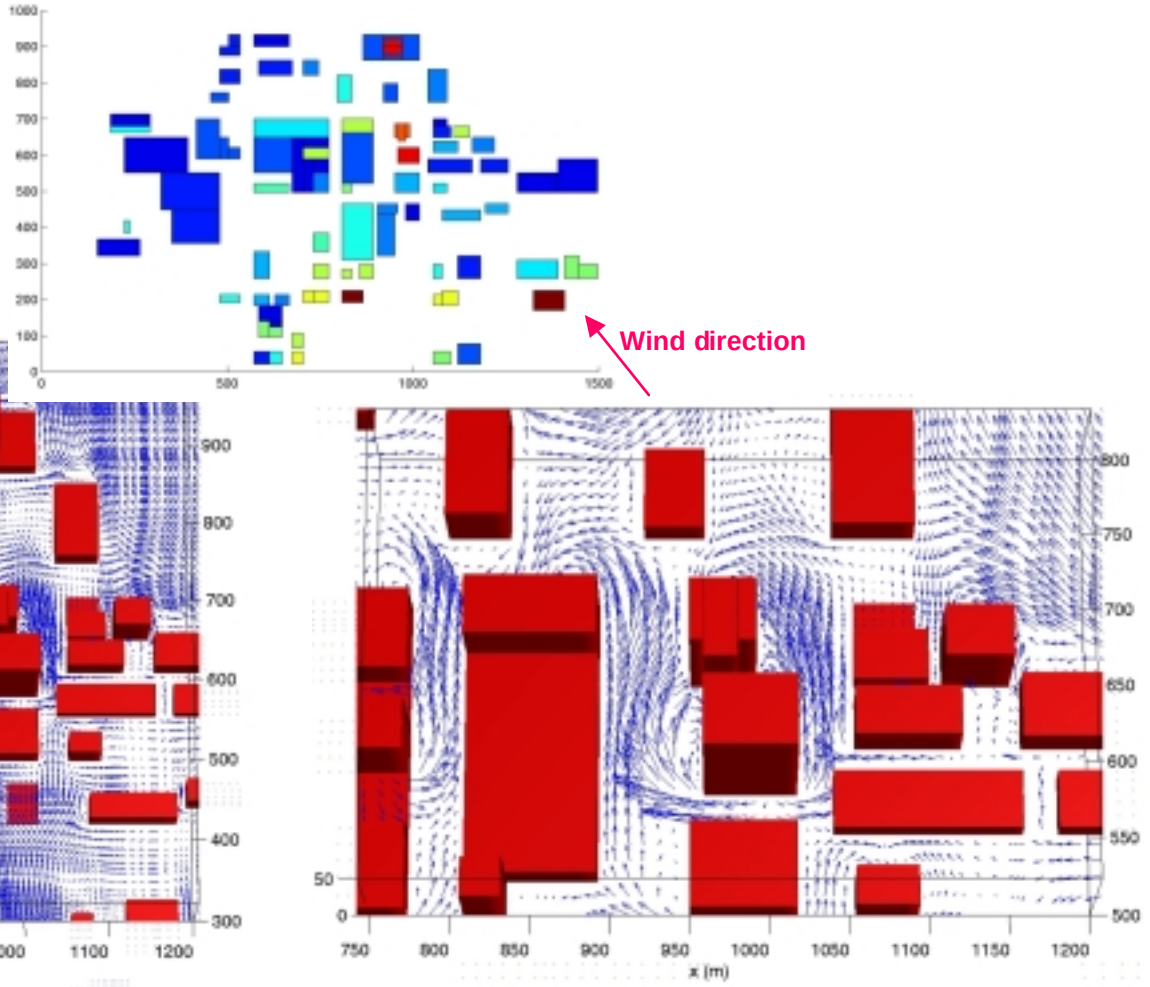
WE ARE DEVELOPING A GRID NESTING CAPABILITY IN SUPPORT OF CBNP's SALT LAKE CITY FIELD EXPERIMENTS



HORIZONTAL CROSS-SECTIONS OF THE WIND FIELD AT 10 m ABOVE SURFACE

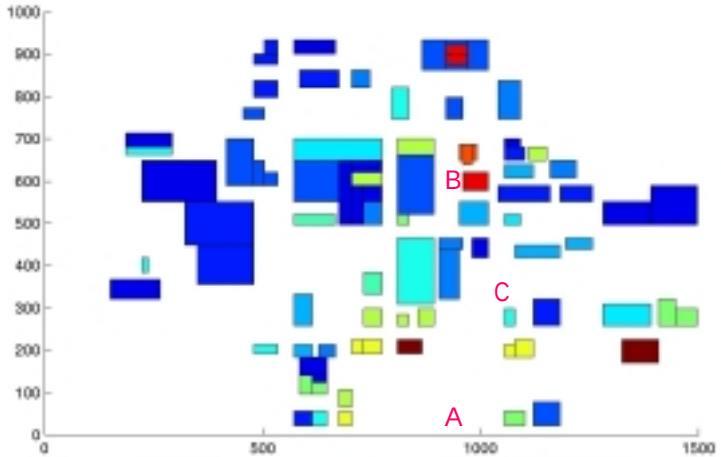


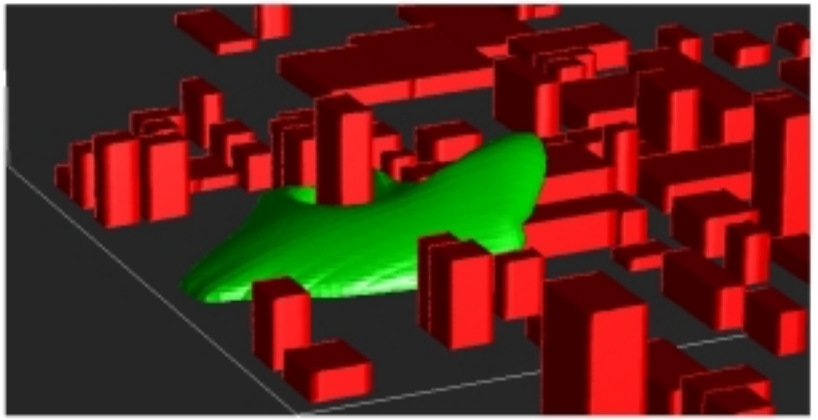
Wind pattern around downtown office complex



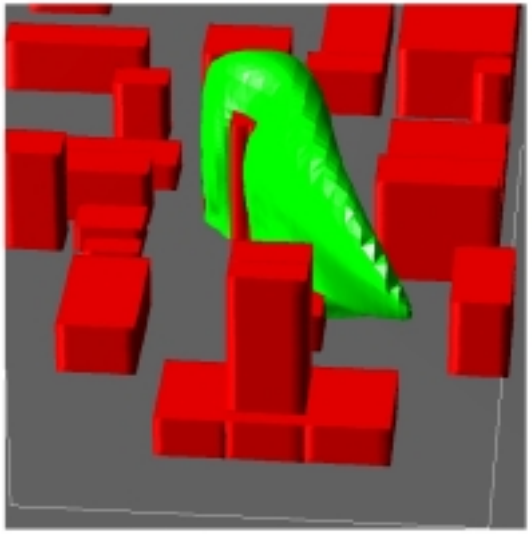
Close-in wind pattern around office towers

DISPERSION PATTERNS FOR SURFACE RELEASES AT VARIOUS DOWNTOWN LOCATIONS AT 300s AFTER RELEASE

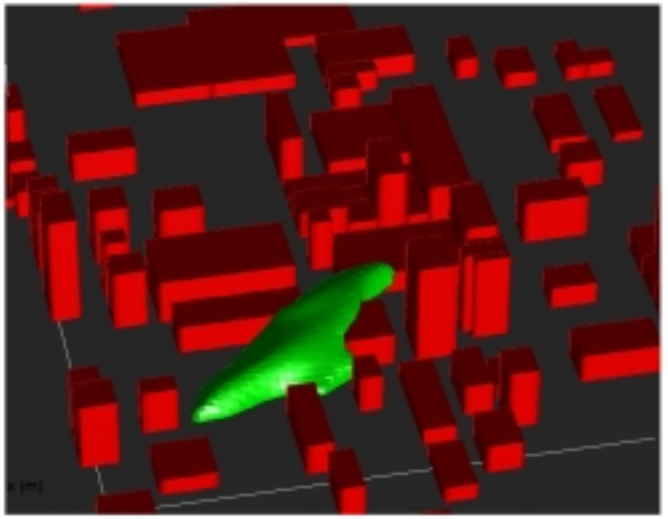




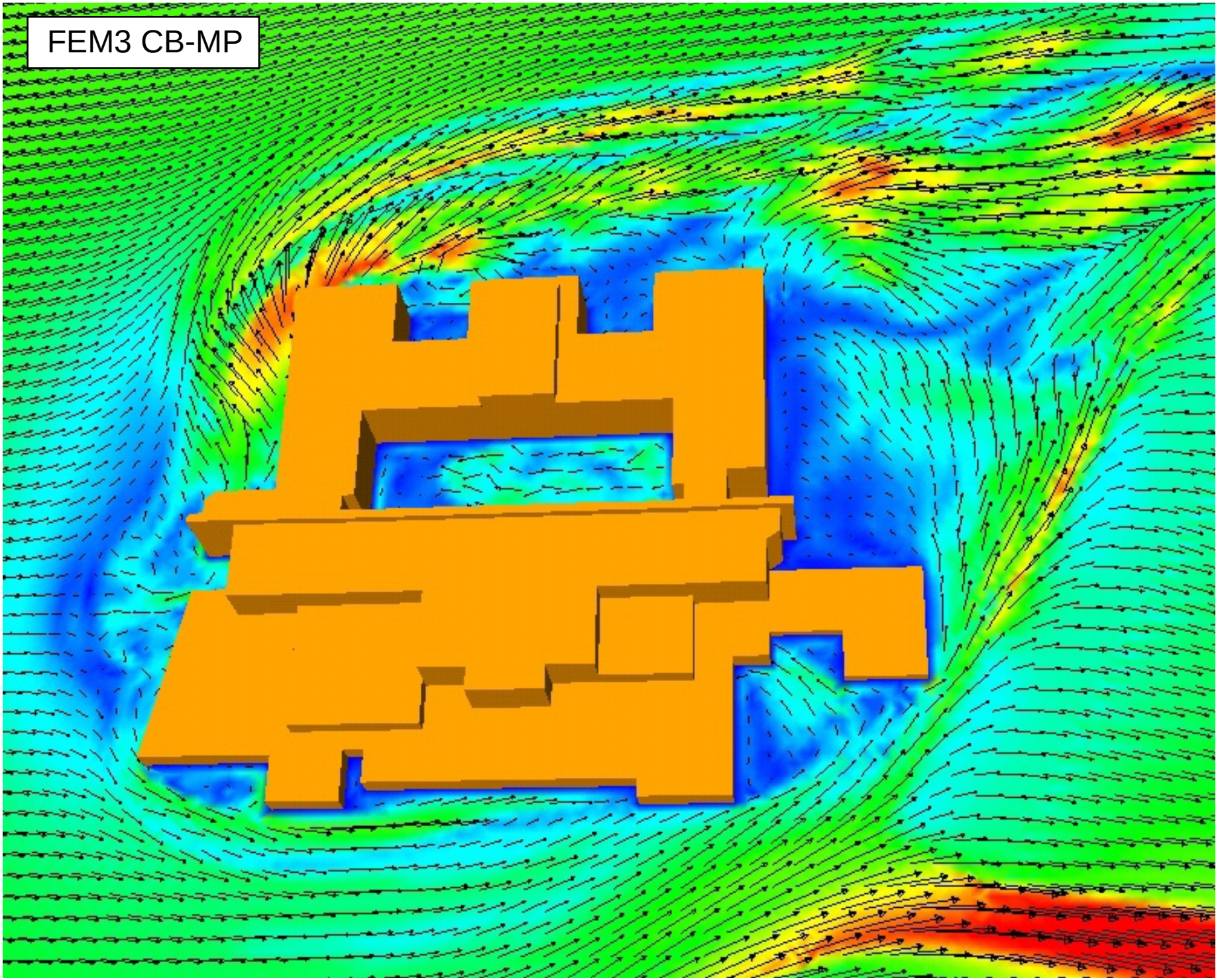
Release south of downtown (A)



Release in front of Mormon office tower (B)

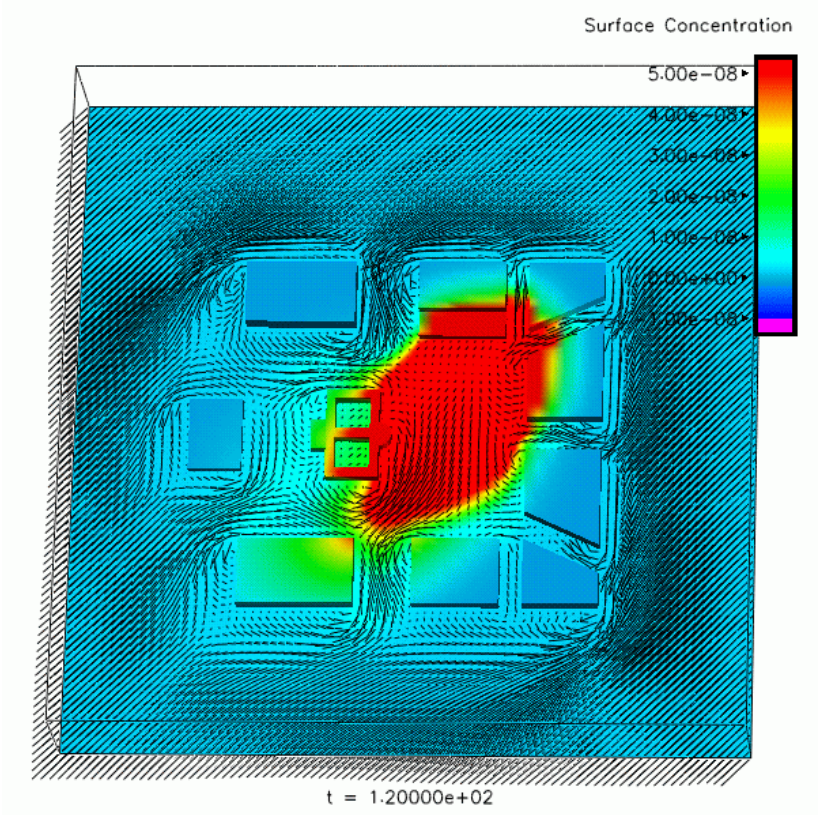


Release southeast of downtown (C)

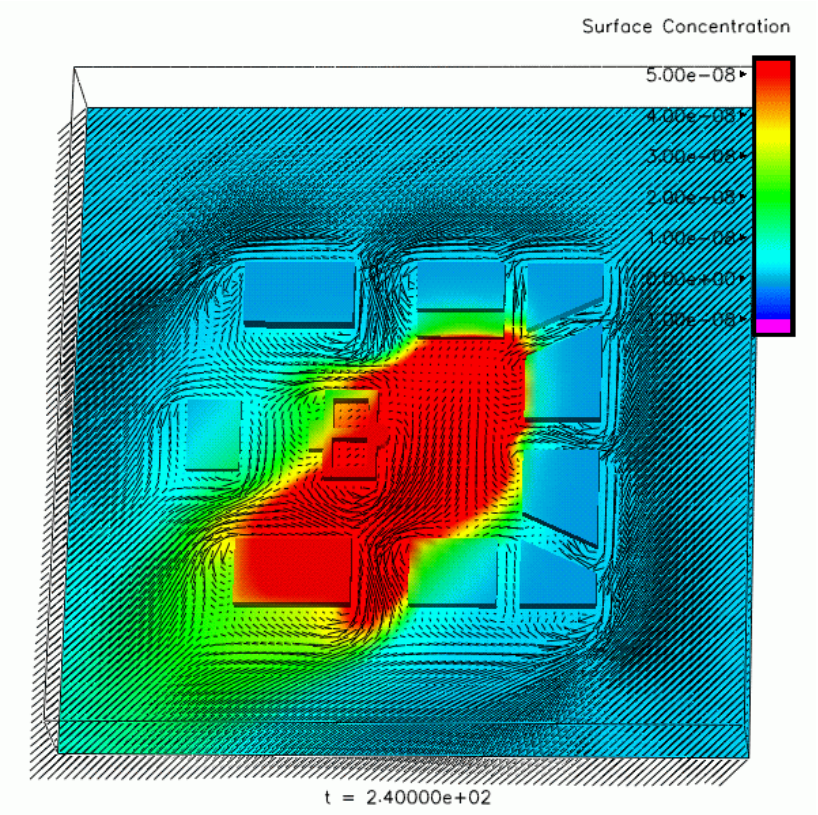

FEM3 CB-MP

BUILDING SCALE DISPERSION SIMULATION

FEM3 CB-MP



Surface concentration pattern at t = 120 s



Surface concentration pattern at t = 240 s